

Supplementary Material for  
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**Synthesis, conformational parameters and packing  
considerations of methyl bispyridyl ketones**

Christian Weck, Felix Katzsch, Tobias Gruber\*

*Institute of Organic Chemistry, Technische Universität Bergakademie Freiberg,  
Leipziger Strasse 29, Freiberg/Sachsen, Germany;*

*Email: Tobias.Gruber@chemie.tu-freiberg.de*

**Table S1**  
Geometrical parameters (Å, °) for compound **2**

N2-C8 = 1.3390(18)	N4-C25 = 1.3418(17)
N2-C12 = 1.3444(18)	N4-C21 = 1.3449(17)
C1-C2 = 1.3848(19)	C14-C15 = 1.3843(18)
C1-C7 = 1.4920(19)	C14-C20 = 1.4939(18)
C2-C3 = 1.377(2)	C15-C16 = 1.387(2)
C2-H2 = 0.9300	C15-H15 = 0.9300
C3-C4 = 1.380(2)	C16-C17 = 1.376(2)
C3-H3 = 0.9300	C16-H16 = 0.9300
C4-C5 = 1.3973(19)	C17-C18 = 1.392(2)
C4-H4 = 0.9300	C17-H17 = 0.9300
C5-C6 = 1.4974(19)	C18-C19 = 1.4978(19)
C6-H6A = 0.9600	C19-H19A = 0.9600
C6-H6B = 0.9600	C19-H19B = 0.9600
C6-H6C = 0.9600	C19-H19C = 0.9600
C7-C8 = 1.4998(19)	C20-C21 = 1.4979(18)
C8-C9 = 1.382(2)	C21-C22 = 1.3869(19)
C9-C10 = 1.380(2)	C22-C23 = 1.3847(19)
C9-H9 = 0.9300	C22-H22 = 0.9300
C10-C11 = 1.377(2)	C23-C24 = 1.379(2)
C10-H10 = 0.9300	C23-H23 = 0.9300
C11-C12 = 1.389(2)	C24-C25 = 1.396(2)
C11-H11 = 0.9300	C24-H24 = 0.9300
C12-C13 = 1.498(2)	C25-C26 = 1.4964(19)
C13-H13A = 0.9600	C26-H26A = 0.9600
C13-H13B = 0.9600	C26-H26B = 0.9600
C13-H13C = 0.9600	C26-H26C = 0.9600
C5-N1-C1 = 117.66(11)	C18-N3-C14 = 117.28(11)
C8-N2-C12 = 117.29(12)	C25-N4-C21 = 117.34(11)
N1-C1-C2 = 124.05(12)	N3-C14-C15 = 124.44(12)
N1-C1-C7 = 115.99(11)	N3-C14-C20 = 116.14(11)
C2-C1-C7 = 119.73(12)	C15-C14-C20 = 119.28(12)
C3-C2-C1 = 117.81(13)	C14-C15-C16 = 117.64(13)
C3-C2-H2 = 121.1	C14-C15-H15 = 121.2
C1-C2-H2 = 121.1	C16-C15-H15 = 121.2
C2-C3-C4 = 119.32(13)	C17-C16-C15 = 118.56(13)
C2-C3-H3 = 120.3	C17-C16-H16 = 120.7
C4-C3-H3 = 120.3	C15-C16-H16 = 120.7
C3-C4-C5 = 119.48(13)	C16-C17-C18 = 120.28(13)
C3-C4-H4 = 120.3	C16-C17-H17 = 119.9
C5-C4-H4 = 120.3	C18-C17-H17 = 119.9
N1-C5-C4 = 121.64(12)	N3-C18-C17 = 121.69(13)
N1-C5-C6 = 116.65(12)	N3-C18-C19 = 117.19(12)
C4-C5-C6 = 121.71(12)	C17-C18-C19 = 121.10(12)
C5-C6-H6A = 109.5	C18-C19-H19A = 109.5

C5-C6-H6B = 109.5  
 H6A-C6-H6B = 109.5  
 C5-C6- H6C = 109.5  
 H6A-C6-H6C = 109.5  
 H6B-C6-H6C = 109.5  
 O1-C7-C1 = 120.65(13)  
 O1-C7-C8 = 119.60(12)  
 C1-C7-C8 = 119.66(11)  
 N2-C8-C9 = 124.13(13)  
 N2-C8-C7 = 116.84(12)  
 C9-C8-C7 = 118.97(13)  
 C10-C9-C8 = 117.98(14)  
 C10-C9-H9 = 121.0  
 C8-C9-H9 = 121.0  
 C11-C10-C9 = 118.86(14)  
 C11-C10-H10 = 120.6  
 C9-C10-H10 = 120.6  
 C10-C11-C12 = 119.70(14)  
 C10-C11-H11 = 120.1  
 C12-C11-H11 = 120.1  
 N2-C12-C11 = 121.95(13)  
 N2-C12-C13 = 116.49(13)  
 C11-C12-C13 = 121.56(13)  
 C12-C13-H13A = 109.5  
 C12-C13-H13B = 109.5  
 H13A-C13-H13B = 109.5  
 C12-C13-H13C = 109.5  
 H13A-C13-H13C = 109.5  
 H13B-C13-H13C = 109.5  
  
 C5-N1-C1-C2 = 1.47(19)  
 C5-N1-C1-C7 = -173.03(11)  
 N1-C1-C2-C3 = -0.3(2)  
 C7-C1-C2-C3 = 174.02(12)  
 C1-C2-C3-C4 = -1.4(2)  
 C2-C3-C4-C5 = 1.8(2)  
 C1-N1-C5-C4 = -0.98(19)  
 C1-N1-C5-C6 = 178.73(11)  
 C3-C4-C5-N1 = -0.6(2)  
 C3-C4-C5-C6 = 179.67(13)  
 N1-C1-C7-O1 = 153.09(13)  
 C2-C1-C7-O1 = -21.67(19)  
 N1-C1-C7-C8 = -23.48(17)  
 C2-C1-C7-C8 = 161.76(12)  
 C12-N2-C8-C9 = 1.8(2)  
 C12-N2-C8-C7 = -175.30(12)  
 O1-C7-C8-N2 = 123.04(14)

C18-C19-H19B = 109.5  
 H19A-C19-H19B = 109.5  
 C18-C19-H19C = 109.5  
 H19A-C19-H19C = 109.5  
 H19B-C19-H19C = 109.5  
 O2-C20-C14 = 120.38(12)  
 O2-C20-C21 = 119.78(12)  
 C14-C20-C21 = 119.83(11)  
 N4-C21-C22 = 124.17(12)  
 N4-C21-C20 = 116.44(11)  
 C22-C21-C20 = 119.32(12)  
 C23-C22-C21 = 117.79(13)  
 C23-C22-H22 = 121.1  
 C21-C22-H22 = 121.1  
 C24-C23-C22 = 118.98(13)  
 C24-C23-H23 = 120.5  
 C22-C23-H23 = 120.5  
 C23-C24-C25 = 119.67(13)  
 C23-C24-H24 = 120.2  
 C25-C24-H24 = 120.2  
 N4-C25-C24 = 121.99(13)  
 N4-C25-C26 = 116.91(12)  
 C24-C25-C26 = 121.10(12)  
 C25-C26-H26A = 109.5  
 C25-C26-H26B = 109.5  
 H26A-C26-H26B = 109.5  
 C25-C26-H26C = 109.5  
 H26A-C26-H26C = 109.5  
 H26B-C26-H26C = 109.5  
  
 C18-N3-C14-C15 = 0.95(19)  
 C18-N3-C14-C20 = -174.78(11)  
 N3-C14-C15-C16 = 1.8(2)  
 C20-C14-C15-C16 = 177.45(12)  
 C14-C15-C16-C17 = -2.3(2)  
 C15-C16-C17-C18 = 0.1(2)  
 C14-N3-C18-C17 = -3.28(18)  
 C14-N3-C18-C19 = 175.70(11)  
 C16-C17-C18-N3 = 2.8(2)  
 C16-C17-C18-C19 = -176.11(13)  
 N3-C14-C20-O2 = 140.14(13)  
 C15-C14-C20-O2 = -35.83(19)  
 N3-C14-C20-C21 = -39.05(16)  
 C15-C14-C20-C21 = 144.98(12)  
 C25-N4-C21-C22 = 1.17(18)  
 C25-N4-C21-C20 = -175.78(11)  
 O2-C20-C21-N4 = 141.12(13)

C1-C7-C8-N2 = -60.36(16)	C14-C20-C21-N4 = -39.68(16)
O1-C7-C8-C9 = -54.21(18)	O2-C20-C21-C22 = -35.98(18)
C1-C7-C8-C9 = 122.39(14)	C14-C20-C21-C22 = 143.22(12)
N2-C8-C9-C10 = 0.8(2)	N4-C21-C22-C23 = 1.18(19)
C7-C8-C9-C10 = 177.80(13)	C20-C21-C22-C23 = 178.04(12)
C8-C9-C10-C11 = -2.7(2)	C21-C22-C23-C24 = -2.07(19)
C9-C10-C11-C12 = 2.2(2)	C22-C23-C24-C25 = 0.7(2)
C8-N2-C12-C11 = -2.38(19)	C21-N4-C25-C24 = -2.62(18)
C8-N2-C12-C13 = 178.57(12)	C21-N4-C25-C26 = 178.13(11)
C10-C11-C12-N2 = 0.4(2)	C23-C24-C25-N4 = 1.7(2)
C10-C11-C12-C13 = 179.43(14)	C23-C24-C25-C26 = -179.05(13)

**Table S2**  
Geometrical parameters (Å, °) for compound **3**

Br1-C6 = 1.972(2)	C6-H6A = 0.9900
N1-C5 = 1.339(3)	C6-H6B = 0.9900
N1-C1 = 1.340(3)	C7-C8 = 1.502(4)
N2-C12 = 1.345(3)	C8-C9 = 1.391(4)
N2-C8 = 1.348(3)	C9-C10 = 1.384(4)
O1-C7 = 1.219(3)	C9-H9 = 0.9500
C1-C2 = 1.393(4)	C10-C11 = 1.380(4)
C1-C7 = 1.514(3)	C10-H10 = 0.9500
C2-C3 = 1.392(4)	C11-C12 = 1.392(4)
C2-H2 = 0.9500	C11-H11 = 0.9500
C3-C4 = 1.378(4)	C12-C13 = 1.503(4)
C3-H3 = 0.9500	C13-H13A = 0.9800
C4-C5 = 1.399(3)	C13-H13B = 0.9800
C4-H4 = 0.9500	C13-H13C = 0.9800
C5-C6 = 1.495(3)	
C5-N1-C1 = 117.6(2)	O1-C7-C1 = 119.9(2)
C12-N2-C8 = 117.7(2)	C8-C7-C1 = 119.8(2)
N1-C1-C2 = 123.6(2)	N2-C8-C9 = 123.7(2)
N1-C1-C7 = 114.5(2)	N2-C8-C7 = 117.4(2)
C2-C1-C7 = 121.8(2)	C9-C8-C7 = 118.9(2)
C3-C2-C1 = 118.2(2)	C10-C9-C8 = 118.1(3)
C3-C2-H2 = 120.9	C10-C9-H9 = 120.9
C1-C2-H2 = 120.9	C8-C9-H9 = 120.9
C4-C3-C2 = 118.8(2)	C11-C10-C9 = 118.7(2)
C4-C3-H3 = 120.6	C11-C10-H10 = 120.7
C2-C3-H3 = 120.6	C9-C10-H10 = 120.7
C3-C4-C5 = 119.2(2)	C10-C11-C12 = 120.2(3)
C3-C4-H4 = 120.4	C10-C11-H11 = 119.9
C5-C4-H4 = 120.4	C12-C11-H11 = 119.9

N1-C5-C4 = 122.5(2)  
N1-C5-C6 = 116.2(2)  
C4-C5-C6 = 121.3(2)  
C5-C6-Br1 = 111.04(17)  
C5-C6-H6A = 109.4  
Br1-C6-H6A = 109.4  
C5-C6-H6B = 109.4  
Br1-C6-H6B = 109.4  
H6A-C6-H6B = 108.0  
O1-C7-C8 = 120.3(2)

C5-N1-C1-C2 = -1.1(4)  
C5-N1-C1-C7 = -177.7(2)  
N1-C1-C2-C3 = -2.0(4)  
C7-C1-C2-C3 = 174.3(2)  
C1-C2-C3-C4 = 2.3(4)  
C2-C3-C4-C5 = 0.4(4)  
C1-N1-C5-C4 = 4.0(4)  
C1-N1-C5-C6 = -173.5(2)  
C3-C4-C5-N1 = -3.7(4)  
C3-C4-C5-C6 = 173.7(2)  
N1-C5-C6-Br1 = -83.4(2)  
C4-C5-C6-Br1 = 99.1(2)  
N1-C1-C7-O1 = 33.9(3)  
C2-C1-C7-O1 = -142.8(2)  
N1-C1-C7-C8 = -146.9(2)

N2-C12-C11 = 121.7(2)  
N2-C12-C13 = 116.5(2)  
C11-C12-C13 = 121.8(2)  
C12-C13-H13A = 109.5  
C12-C13-H13B = 109.5  
H13A-C13-H13B = 109.5  
C12-C13-H13C = 109.5  
H13A-C13-H13C = 109.5  
H13B-C13-H13C = 109.5

C2-C1-C7-C8 = 36.5(3)  
C12-N2-C8-C9 = 0.1(4)  
C12-N2-C8-C7 = 178.7(2)  
O1-C7-C8-N2 = -155.2(2)  
C1-C7-C8-N2 = 25.6(3)  
O1-C7-C8-C9 = 23.5(4)  
C1-C7-C8-C9 = -155.8(2)  
N2-C8-C9-C10 = -0.6(4)  
C7-C8-C9-C10 = -179.1(2)  
C8-C9-C10-C11 = 0.4(4)  
C9-C10-C11-C12 = 0.2(4)  
C8-N2-C12-C11 = 0.4(4)  
C8-N2-C12-C13 = -179.8(2)  
C10-C11-C12-N2 = -0.6(4)  
C10-C11-C12-C13 = 179.7(3)

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